

Technology Opportunity

Thermochemical Properties of Species and Mixtures

The National Aeronautics and Space Administration (NASA) seeks industrial partners to develop, transfer, and license computer codes that predict the thermodynamic and kinetic behavior of equilibrium and nonequilibrium mixtures over a wide range of temperatures, pressures, and compositions.

Potential Commercial Uses

- Optimizing the design of manufacturing and material handling equipment
- Computationally calibrating flow control devices
- Predicting the performance of combustion systems (efficiency and emissions)

Benefits

- User friendly, efficient state-of-the-art computer codes
- Critically reviewed databases
- Custom optimization of the codes for specific user application

The Technology

Understanding and predicting the thermodynamic and kinetic behavior of chemical mixtures is important in many manufacturing and control applications. The NASA Lewis Research Center's family of computer codes (PAC, Properties and Coefficients; CEA, Chemical Equilibrium and Applications; and LSENS, Lewis Kinetics and Sensitivity Analysis) enables the user to accurately predict the response of a bulk mixture to a number of external stimuli (e.g., compression, heating, and chemical reaction). The codes have a user friendly input and can accommodate a large variety of conditions. The databases for the thermochemical calculations consist

of a series of polynomials for individual species. These polynomials are developed through critical review of the available literature augmented by quantum chemical and other estimation techniques where literature data are lacking. User specific requirements and conditions can be added on an ad hoc basis.

Options for Commercialization

Seeking to license technology. Seeking partnership with industry to develop and transfer technology.

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Key Words

Thermodynamics
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Transport
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